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Quantum-Confined Hole States in Double-Barrier Resonant Tunneling Structures

by

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Abstract

Double-barrier resonant tunneling structures often contain undoped spacer layers separating heavily *n*-doped regions from active regions of the structure. Conduction band electrons coming from the heavily doped regions diffuse into the undoped regions, producing potential energy profiles that can confine hole states within the spacer layers. A classical model is used to predict the potential energy profiles in these structures, and the associated hole binding energies and wave functions are calculated numerically.

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1. Introduction

Double-barrier resonant tunneling (DBRT) structures (and in fact a variety of different semiconductor heterostructures) often contain heavily doped regions and undoped "active" regions separated by an undoped spacer layer. Attempts to model the electronic states in these structures always involve assumptions regarding the distribution of extended-state electrons (or holes) near the abrupt doping profile edge.[1] For example, *n*-type DBRT structures often contain undoped spacer layers (about 100 Å thick) surrounding the barrier/quantum-well (QW) region of the structure. These layers are in turn surrounded by heavily *n*-doped regions that facilitate electrical contact to the sample. The present paper deals with the nature of the band-bending near spacer layers and the hole states that are confined (in one spatial dimension) by this space-charge potential.

We use a classical model of the charge distribution to derive expressions for the potential profile in unbiased DBRT structures. We then integrate a one-band effective mass Schrödinger equation through the region of interest to obtain the hole states confined by the potential. In a concluding section, we comment on the classical model's weakness and indicate how the theory might be improved so that the potential profile and binding energy estimates are more reliable.

2. Model and Calculations

Consider the energy band diagram of a typical DBRT structure, shown in figure 1. The host semiconductor might be GaAs and the barrier layers AlGaAs. We assume that the region between the vertical dotted lines is undoped while the region outside the dotted lines is uniformly doped. We further assume for simplicity that all donor atoms are ionized and that the electrons associated with them occupy extended conduction band states. In modeling the free electron distribution in this structure, we replace the discrete, randomly distributed ionized donor atoms by a uniform positive background, and we ignore potential fluctuations. We now ask, how do the

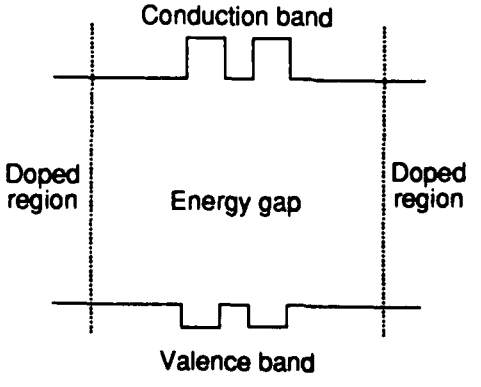

Figure 1. Energy band diagram of a double-barrier resonant tunneling structure. Region between vertical dotted lines is undoped.

[1] *See, for example, models described in T. Ando, A. Fowler, and F. Stern, Rev. Mod. Phys. 54, 437 (1982).*

electrons distribute themselves in the presence of this background charge density? We address this question from a classical point of view, commenting later on improvements to the model.

At $T = 0$ K, the electron charge density will perfectly match the positive background charge density, and the electrostatic potential will be zero everywhere. At a finite temperature, some electrons will diffuse into the undoped region (on a distance scale comparable to a Debye length) leading to dipole layers centered near the doping edges. This will produce an electrostatic potential that decreases as one enters the undoped region from either side of the structure (fig. 1 corresponds to this classical picture at zero temperature). Let $z = 0$ correspond to the doping edge on the left side of figure 1 (vertical dotted line), with z increasing towards the double-barrier structure. We take the spacer layer to have a thickness t and assume that electron density is zero inside the barrier and QW regions of the structure.* This implies that electrons which diffuse past the doping edge must reside in the spacer-layer region, and therefore, the electric field at $z = t$ is zero.

In the classical approach to the problem, the electron number density $n(z)$ is given by

$$n(z) = n_d \exp[\beta e \phi(z)] \ , \tag{1}$$

where $\beta = 1/kT$, n_d is the donor density, e is the electronic charge, and $\phi(z)$ is the electrostatic potential (assumed equal to zero at $z = -\infty$). Expression (1) is readily obtained by assuming that (a) $\phi(z)$ changes slowly enough that, at any point z, the density of conduction band states is what one would have in a bulk semiconductor (without an electric field) whose band-edge has been shifted by the local value of the potential energy ($-e\phi(z)$), (b) the chemical potential satisfies the inequality $E_c - e\phi(z) - \mu >> kT$, where E_c is the conduction-band-edge energy, and (c) $n(z)$ is always much greater than the intrinsic charge density in the conduction band. The first two assumptions will not be satisfied for some choices of n_d, T, and t. In particular, assumption (b) is certainly violated over some region of the structure for degenerately doped materials. Nevertheless, corrections due to electron degeneracy are sometimes minor and, as a first estimate of the potential profile and hole-binding energies, the nondegenerate result will suffice. Next we impose the requirement that Poisson's equation be satisfied:

$$\frac{d^2\phi(z)}{dz^2} = -\frac{4\pi\rho(z)}{\varepsilon} \ , \tag{2}$$

where ε is the static dielectric constant of the host semiconductor, and $\rho(z)$ is given by

$$\rho(z) = \begin{pmatrix} e[n_d - n(z)] & \text{for } z < 0 \\ -en(z) & \text{for } z > 0 \end{pmatrix} . \tag{3}$$

*We assume that the barrier height is infinite.

By combining equations (1), (2), and (3), one obtains the equations

$$\frac{d^2U(z)}{dz^2} = -\frac{1}{l^2}\exp[-U(z)] \qquad \text{for } z>0, \quad \text{and} \tag{4}$$

$$\frac{d^2U(z)}{dz^2} = +\frac{1}{l^2}\left(1-\exp[-U(z)]\right) \qquad \text{for } z<0, \tag{5}$$

where $U(z)$ is a dimensionless potential energy defined by $U(z) = -\beta e\phi(z)$, and l is the classical Debye length given by

$$l = \left(\frac{\varepsilon k_B T}{4\pi n_d e^2}\right)^{1/2} . \tag{6}$$

Equation (4) can be integrated analytically to obtain, for the $z > 0$ region,

$$U(z) = U(t) + 2\ln\left[\cos\left(\theta_0 - \frac{\exp[-U(t)/2]z}{\sqrt{2}\,l}\right)\right] , \tag{7}$$

where θ_0 is defined by $\cos^2\theta_0 = \exp(U(0) - U(t))$.

The solution to equation (5) can be given in terms of a definite integral (which cannot itself be profitably expressed in terms of special functions). We obtain, for $z < 0$,

$$U(z) = G^{-1}\left(M[U(0)] + \frac{\sqrt{2}\,z}{l}\right) . \tag{8}$$

The single-valued function G is given by

$$G(x) = M(x) + \sqrt{2}\,\ln[x/U(0)] ,$$

where $M(x)$ is defined by

$$M(x) = \int_0^x dy\left[\frac{1}{\sqrt{y+\exp(-y)-1}} - \frac{\sqrt{2}}{y}\right]. \tag{9}$$

The solutions obtained for differential equations (4) and (5) both require the specification of boundary conditions. We have already implicitly imposed continuity of $U(z)$ at $z = 0$. By requiring that the electric field at $z = 0$ (which is proportional to $U'(0)$) be continuous, we obtain, equating first integrals of (4) and (5),

$$\exp[-U(t)] = 1 - U(0) . \tag{10}$$

Another relation between $U(0)$ and $U(t)$ is obtained by evaluating equation (7) at $z = t$. After combining this second relation with equation (10), we obtain a transcendental equation for $U(t)$, namely,

$$1 - U(t) - \exp[-U(t)] = 2\ln\left[\cos\left(\frac{t\exp[-U(t)/2]}{\sqrt{2}\,l}\right)\right] . \tag{11}$$

This expression contains only one unknown, $U(t)$, which can be found by root-solving. Once $U(t)$ is known, $U(0)$ can be obtained from (10). The results can then be used in the solutions to (4) and (5) to calculate the potential energy function.

We have carried out this procedure and in figure 2a, we plot the valence-band-edge diagram of a DBRT structure at three temperatures: T = 77, 150, and 300 K. Figure 2b shows the depth of the hole-confining potential well as a function of temperature. We have chosen the structure's parameters as follows: t = 150 Å, $n_d = 2 \times 10^{18}$ cm^{-3}, 150-meV AlGaAs barrier height, 42.25-Å QW width, and 62.5-Å barrier width (the latter three are irrelevant for the calculation of the potential). We now integrate a one-band effective mass Schrödinger equation through the spacer-layer region of the structure. In figures 3a and 3b, we plot the T = 300 K hole-confining potential (upside down and reversed) along with the confined heavy- and light-hole wave functions, respectively. Figures 3c and 3d contain similar results at T = 77 K. The wave functions are labelled by the binding energies. These results were obtained by numerically integrating a one-band effective-mass Schrödinger equation for $\psi(x)$ ($x \equiv t - z$), subject to the requirement that $\psi(x)$ go to zero far inside the barrier region ($x << 0$) and far inside the doped region ($x >> t$), and that ψ'/m^* be continuous at the barrier interface (where m^* is the hole effective mass). In our calculations, we used $m_{hh} = 0.34\ m_0$ and $m_{lh} = 0.094\ m_0$ for the heavy- and light-hole masses in the host semiconductor, and $m_{hh} = 0.433\ m_0$ and $m_{lh} = 0.109\ m_0$ for heavy- and light-hole masses in the barrier layer (values which correspond to an Al fraction of about 30 percent).

We believe that if electron-hole pairs were generated within a diffusion length of the doping edge, holes could readily migrate into the spacer layer region, occupying the lowest hole subband calculated above. One would then expect to see luminescence radiation resulting from transitions between extended-state conduction band states and the lowest hole subband, and (maybe) between conduction band DBRT resonance states and the lowest hole

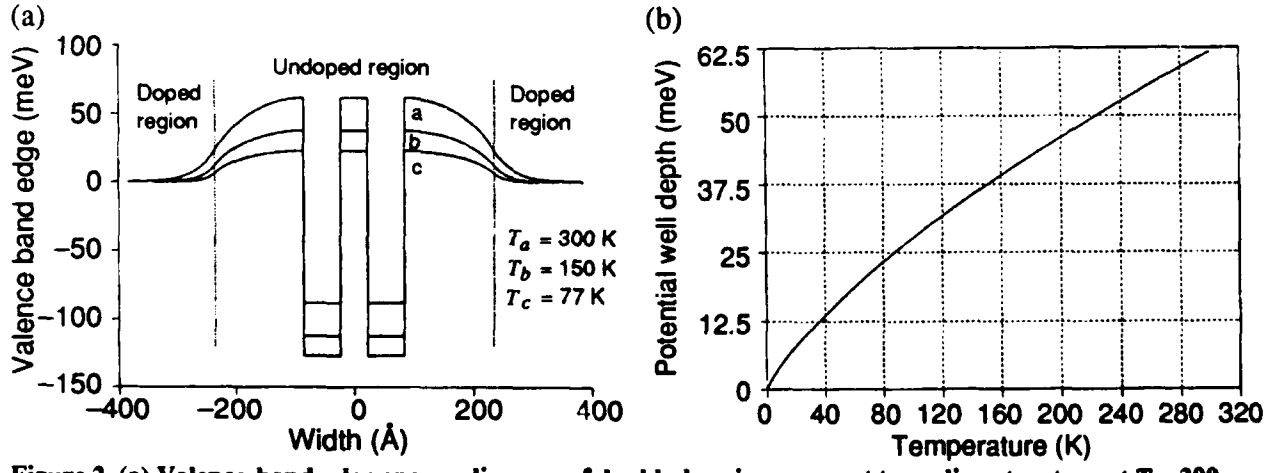

Figure 2. (a) Valence-band-edge energy diagram of double-barrier resonant tunneling structure at T = 300, 150, and 77 K. Spacer layers are 150 Å thick, and doping density of n-doped regions is 2×10^{18} cm^{-3}. (b) Hole-confining potential well depth versus temperature for structure with same parameters.

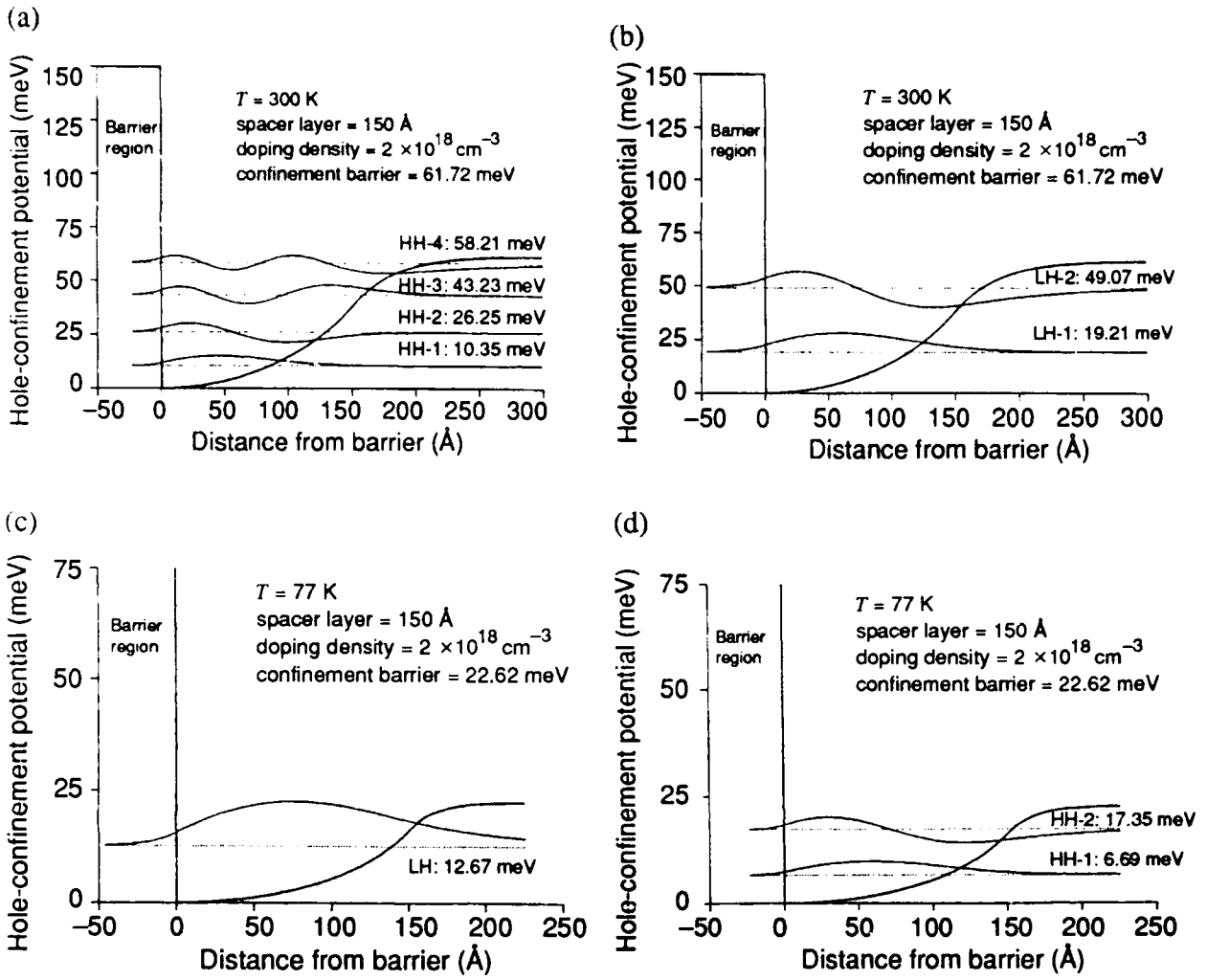

Figure 3. Hole-confining potentials (upside down) plotted with bound heavy- and light-hole wave functions: (a) heavy- and (b) light-hole states at $T = 300$ K; (c) heavy- and (d) light-hole states at $T = 77$ K.

subband. However, seeing such features might prove difficult. The larger binding energies (which are most easily separable from direct-gap-related features in luminescence) occur in the deeper wells, which in turn occur at the higher temperatures (according to the classical picture described above). On the other hand, the higher the temperature, the broader are the photoluminescence line shapes, particularly in heavily doped samples. We believe that one should see, at least, a luminescence band associated with transitions between the low-energy conduction band-edge states and the confined lowest-subband heavy-hole state. We have not calculated the expected position (or shape) of such a band as a function of temperature but believe that it mignt have a characteristic temperature dependence arising from the temperature dependence of the quantum confining potential in the spacer layer. We have made some preliminary piezoreflectance measurements on a DBRT sample (with parameters identical to those used in the model),[2] but have not seen any

[2] *R. L. Tober and J. D. Bruno, Proc. SPIE 1286 (in press).*

convincing evidence of the quantum-confined hole states in the spectra. The experimental effort is still in progress.

3. Conclusions

The assumptions upon which the classical model relies are not well satisfied. We have ignored quantum-mechanical effects in determining the distribution of conduction-band electrons. We then used the very potential obtained from the resulting electron distribution in an effective-mass Schrödinger equation to determine quantum-confined hole states. Our rationale for doing this rested on the lack of a confining potential for electrons. We therefore assumed that the local density of electron states was modified less by the potential than was the local density of hole states. This rationale, however, is not very satisfying. Furthermore, one can expect that even at zero temperature, where the classical picture leads to no potential energy profile, one would have a quantum-mechanical dipole layer, since the electron density cannot drop from n_d to zero on a length scale shorter than λ_F. Here λ_F is the Fermi wavelength of the degenerate electron gas inside the doped regions of the structure. A "back of the envelope" calculation based on this idea leads to a quantum mechanical potential well in the positive background region of the structure whose depth is comparable to the depth of the thermally induced space-charge well seen by holes at room temperature. This implies that a full quantum-mechanical treatment might be required in order to obtain reliable space-charge fields (and hole binding energies) in these DBRT and similar structures. A less important approximation involved replacing the Fermi distribution by a Boltzmann distribution to obtain equation (1). Although conditions required for this approximation's validity are violated to some extent in the structure we considered, corrections due to electron degeneracy are small (in the structure we considered) and do not change the hole binding energies substantially.

In view of the unsatisfactory nature of some approximations made in this work, we are presently applying density functional theory to this problem and will report on that work in the future.

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